**Many-Body Correlations**

We’re often interested in studying correlations in many body systems. So we’ll take some time to define a few…

**Correlation functions in terms of the many body wavefunction**

Getting a little ahead of ourselves, consider the many-body density matrix in the canonical ensemble (we’ll talk about it in the statistical mechanics file, and note that this is the same as the *distribution* function that serves as the basis for statistical mechanics, well, at least in the canonical ensemble)



and now dot both sides by two many-body position eigenstates, like this: <r´1,r´2,…,r´N,σ´1,σ´2,…,σ´N||r1,r2,…,rN,σ1,σ2,…,σN>. Then we’ll have the N-particle thermally averaged correlation function:



which is equivalent to the correlation matrix, as far as information content – it’s just the correlation matrix in the spin-position basis. And we can specialize to T = 0, where the only state thermally occupied will be the ground state, where we will remain. Then we’d have:



and dotting both sides,



We could call this the N-particle correlation function. And we can define the N-particle probability density function (dropping the (0) superscript), which is the diagonal terms of the density matrix/correlation function:



We note that the trace of the correlation function is normalized to 1, since:



Averages of a given quantity A(12…N,1,2,…N,1,2,…,N) can be accomplished via:



Or, with primes where I’d rather they be:



If observable A is function only of position and spin operators, then this would simplify to:



Note this probability density function would give the probability of particles being at the given locations/spins, not the density of particles being there. We can define auxiliary density functions, and matrices. The single particle (probability) density function would be defined as the expectation of the average position operator, which is just the density operator over N.



[the spin δ is a Kronecker delta] Basically, it’s the average of the probabilities that any of the particles is at **r**, spin σ regardless of the positions/spins of the other ones. Seems somewhat more intuitive to me to write fσ(**r**) = probability that particle 1, or 2, or 3, …, or N is at position r and spin σ. But this isn’t necessarily normalized to 1. If distribution is symmetric, then this would just reduce to:



And so we have:



We will observe that Σσ∫d3r fσ(r) = 1 so that’s good. If we want the total probability regardless of spin, then we’d do:



The particle density per spin, nσ(x), is just:



So we can say,



and density regardless of spin is of course,



In a homogeneous system with no spin preference we should have



The single particle distribution function is useful for calculating expectations of additive single particle operators. We can introduce the two particle probability density function as well.



This is the average of all of the pair density functions that one can make out of the N particle set (we are including duplicates because we didn’t say i < j, but then the N(N-1) factor accounts for this). Has units of 1/V2. Again, if the probability distribution function is symmetric, then we would expect to find:



and summing/integrating over Σσσ´d3rd3r´ will give us 1. As usual, if we want the position probability density regardless of spin, then we’d just sum over spin,



There is a related function we can introduce, called the pair correlation function, gσσ´(r,r´), which factors out of the pair probability density function the obvious contributions given by the average density of particles at those points – in other words, it is just the correlationy part of the probability for pairs to be in two locations. It’s defined via:



where it appears we use the spin-independent density in the n’s. So g would be unitless. If we only care about position, then



In a translationally invariant, spin-independent (meaning no spin interaction) system we expect it to be independent of spin, and only depend on the difference of the position arguments, and for the density to be independent of position, and so we could say:



where n0 = N/V. Now consider the probability that two particles are within a distance r from each other. Maybe easiest way is to change variables in fσσ´(r,r´) to s = r-r´, and S = (r+r´)/2. Note Jacobian would be 1. With fσσ´(s,S) in hand, we’d integrate over S and that would give us our fσσ´(s) distribution. Then we have:



Now if fσσ´(r,r´) doesn’t depend on S, as would be the case for a homogeneous system, then we just have:



Filling in our expression in terms of g, we have:



It seems the average value of gσσ´ must generally be (1/4)(1 – 1/N), in order for Σσσ´fσσ´ → 1. Typical plots in Mahan show them asymptoting to ½, not ¼. I think they’re renormalizing the g’s. Their conceit is that we start with a spin up and consider the probability a spin up or down is in its vicinity. Then it would seem that this probability should asymptote to (or more like average to) 1, not ½. But this presumes we can start with a spin up particle in the first place. The probability of this event occuring is ½ itself (for say, a system with no magnetic field polarizing the spins). So I think they’re just leaving off the ½, in effect presuming we have identified a spin up, and going from there. Note that if our system is non-interacting, then we expect fσσ´(r,r´) to not depend on position or spin, and since it must sum/integrate to 1, we must have fσσ´(r,r´) = 1/4V2. Applying this equality to our expression above would imply that gσσ´(r-r´) = N(N-1)/4N2 = (1 – 1/N)/4 exactly. Now consider the one particle *correlation* function:



This should have units of 1/V. We can write this in terms of another single particle correlation function (running out of names) Rσσ´(**r**|**r**´), defined as:



And R should be unitless. In a translationally invariant system/spin-independent system, we’d expect this also to depend on only the arguments’ difference:



Note that when rσ = rʹσ´, then we have fσ(**r**). And so in a translationally invariant system, again, we ought to have Rσσ(0) = 1/2. And we could define a two-particle correlation function,



This should have units of 1/V2. Of course when r´´σ´´ = r´σ´ and r´´´σ´´´ = rσ, then we have the two-particle pair probability density function. Not that we’ll find much use for it.

**Correlation Functions in 2nd quantization formalism**

We can put these functions in a 2nd quantization format, where the expectation is against the N-particle ground state (not necessarily non-interacting) – just check out the 2nd quantization file to see how to do this. In particular:



etc., where we’ve averaged at T = 0, i.e., with respect to |Ψ>, since we’ve been dealing with the GS wavefunction so far. Let’s verify. First consider fσ(r). It’s the expectation of (1/N)Σiδ(r-i)δ(σ-i). So it’s a standard one body operator that can be expressed in 2nd quantized notation as:



(the σ apropos the σ’s is a Kronecker delta) Likewise fσσ´(r,r´) is a standard two-body operator 1/N(N-1)·Σi<jδ(r­-i)δ(r´-j)δ(σ-­i)δ(σ´-j), and so it too can be expressed in 2nd quantized notation as:



Don’t know how to get fσ1|σ´1(r1|r´1) or fσ1,σ2|σ´1,σ´2(r1,r2|r´1,r´2) though. Let’s check the last for a non-interacting 2 body wavefunction |kakb>. Ignoring spin (ε = ± for fermions/bosons), then since N = 2, we must have:



and seeing if this is equal to:



Now I’d use Wick’s theorem (later file) to simplify the product. Same colored pairs are contracted. I believe these are the only ones that exist – remember c†c contractions don’t exist – see Wick’s Theorem a couple files up – and these are forced on you if you try all other combinations of full contractions….



So then,



And both terms match. I’m sure this will continue to be true for larger N. Maybe then for general states too? Let’s also check (N = 2):



So via the first equality we have (going to switch to box normalized states):



and now check that this is the same as:



which is:



So this checks out too. I’m wondering if, for an N-body wavefunction, then, we have that:



**Observables from the correlation functions**

Going to ignore spin throughout the following….The utility of defining R and g is that useful observables can be defined most simply in terms of them. So let’s consider some things we can get from these functions. The F. Transform of R(r|r’) gives the momentum distribution function. For consider,



So we have,



(where n0 = N/V, and R(**k**) is the Fourier transform of R(**r**)) which is the number of particles on average in the momentum state *k*. Often, the R(r) function goes to a constant in the large r limit, and so a convenient manipulation, to extend the integral over all space is to write:



Then we can usually safely extend the last integral to cover all space without changing its value appreciably. Now let’s consider the momentum,



where in the last line we employ the indistinguishability of the particles. And now using f = R/V, we have:



Now let’s look at kinetic energy. Could do similarly,



where in the last line we take advantage of the indistinguishability of the coordinates. And using f = R/V, we have:



This looks better as Fourier transform. Let’s say,



So we have:



This also follows straight from the formula for the KE in the 2nd quantization formalism, using KE = Σknkεk, and nk = n0R(k). What about a single particle potential?



and so we have:



What about an interaction potential energy? We can write the potential energy in terms of the two-particle correlation function. Gonna do this a slightly different way:



Then using,



We have:



Presuming a homogeneous system, though, probably couldn’t if there is a single particle potential, we can use:



to say,



and so the potential energy is:



where n0 = N/V.

**Structure Factor**

The structure factor is related to the Fourier transform of the density operator.



(r is a scalar/parameter, but rj is 1st quantized position operator for the particle j), as usual. I think this definition would serve just as well for any set of random particles. But we’ll want the F transform of this:



Note that the Fourier transform multiplies by a factor of V, so we will end up with overall units of N, not n. We may want to find the expectation of this quantity w/r to our wavefunction. This is:



For a homogeneous system, where the probability distribution of the particles is f(1,2,3,..,N) = 1/VN we’d have:



But generalizing beyond the uniform distribution, we may say that the average over all positions of the atoms will give the same result since we expect that the *r* can vary where ever. For instance, if we were dealing with a translationally invariant system of objects, then we’d get this result. Next we’d like to consider the average over a product of two density operators. Consider,



But we’ll want the F transform of this:



Now we want to evaluate the average w/r to our wavefunction:



It helps to go to center of mass coordinates in ri and rj: Rij = (ri + rj)/2, Δrij = ri – rj.



We don’t expect, in a homogeneous system, for the wavefunction against which we’re taking an expectation to have a preference for the location of the pair’s center of mass. Thus we expect this average will give us δq+q´,0. Starting over, then we can say,



And we can separate that bracket into q = 0 and q ≠ 0 terms.



where the last line serves as the definition of the Structure factor.



Going back to the beginning again, we can say,



And so we shall get:



It’s clear S(q) is related to g(q), and this is how they relate:



We can combine the Nδq0 and n0g(q) terms to get:



**Potential Energy in terms of S(k)**

We would also like to relate the pair correlation function to the structure function. We can do this by looking at the potential energy again. So consider the average interaction potential energy, in 2nd quantized formalism.



Probably we can neglect the V2(0) term?

**Time development of structure factor**

Let’s consider the time development of the structure function now. First we define,



This is often a useful form, since we can evaluate the r(t) stuff from a sort of classical mechanics consideration. We could take the Fourier transform.



*Feenberg* presents the following identities:



One implication of these equations is that

